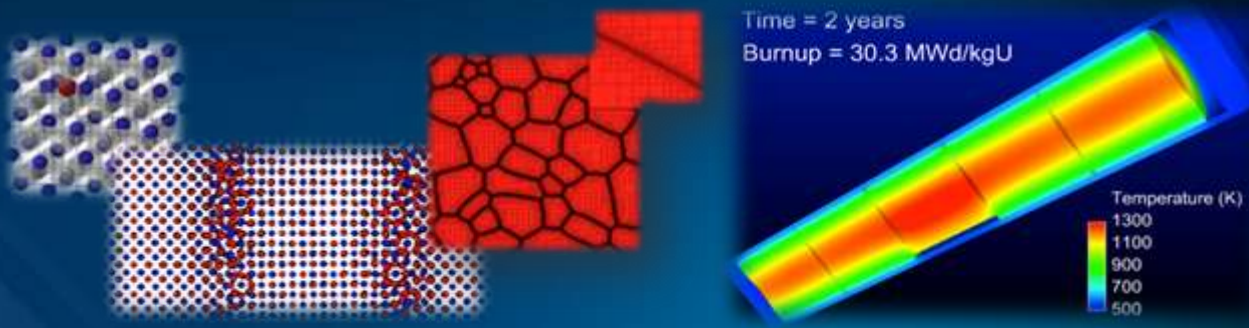
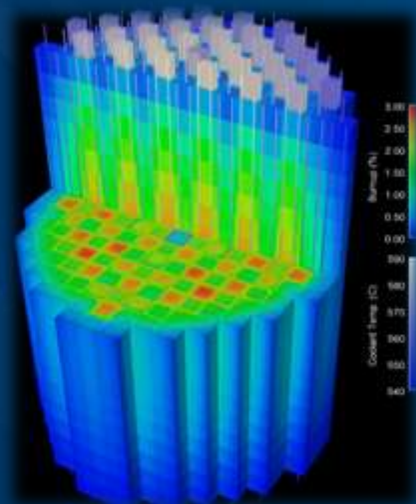
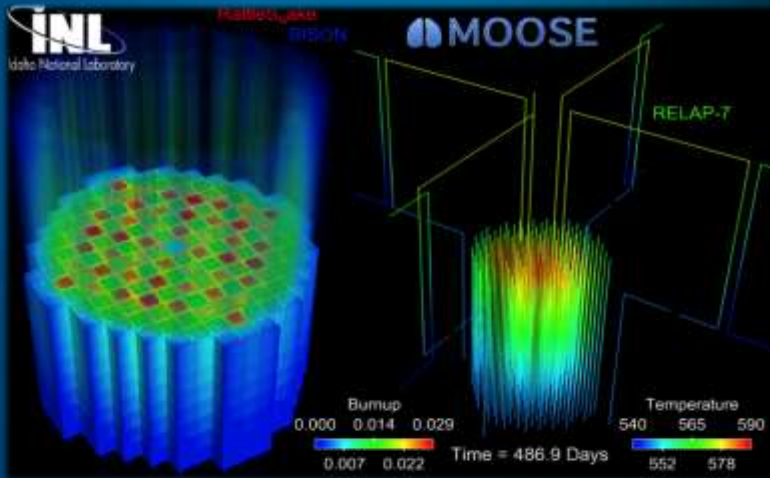
HPC as a Scientific Instrument







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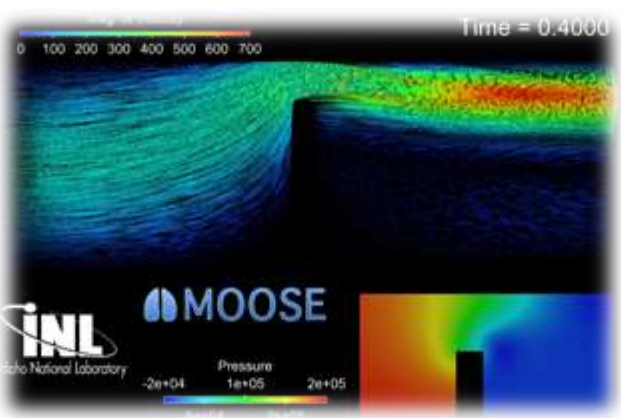
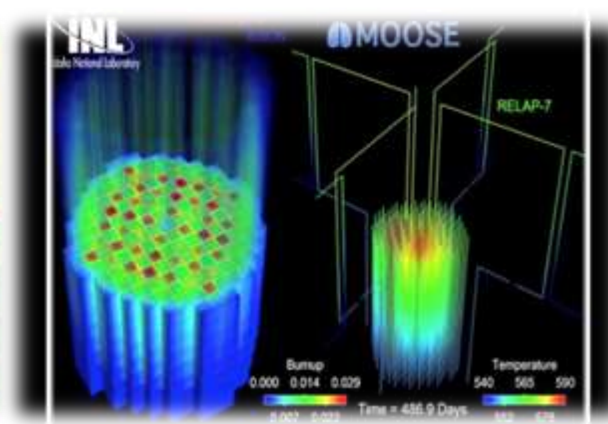
Key Points

- High Performance Computing (HPC) compliments theory and informs experimental processes.
- HPC is a 'microscope' for researchers to better understand physics, chemistry, and engineering principles in ways not otherwise possible.
- People and partnerships are key to success in scientific computing.



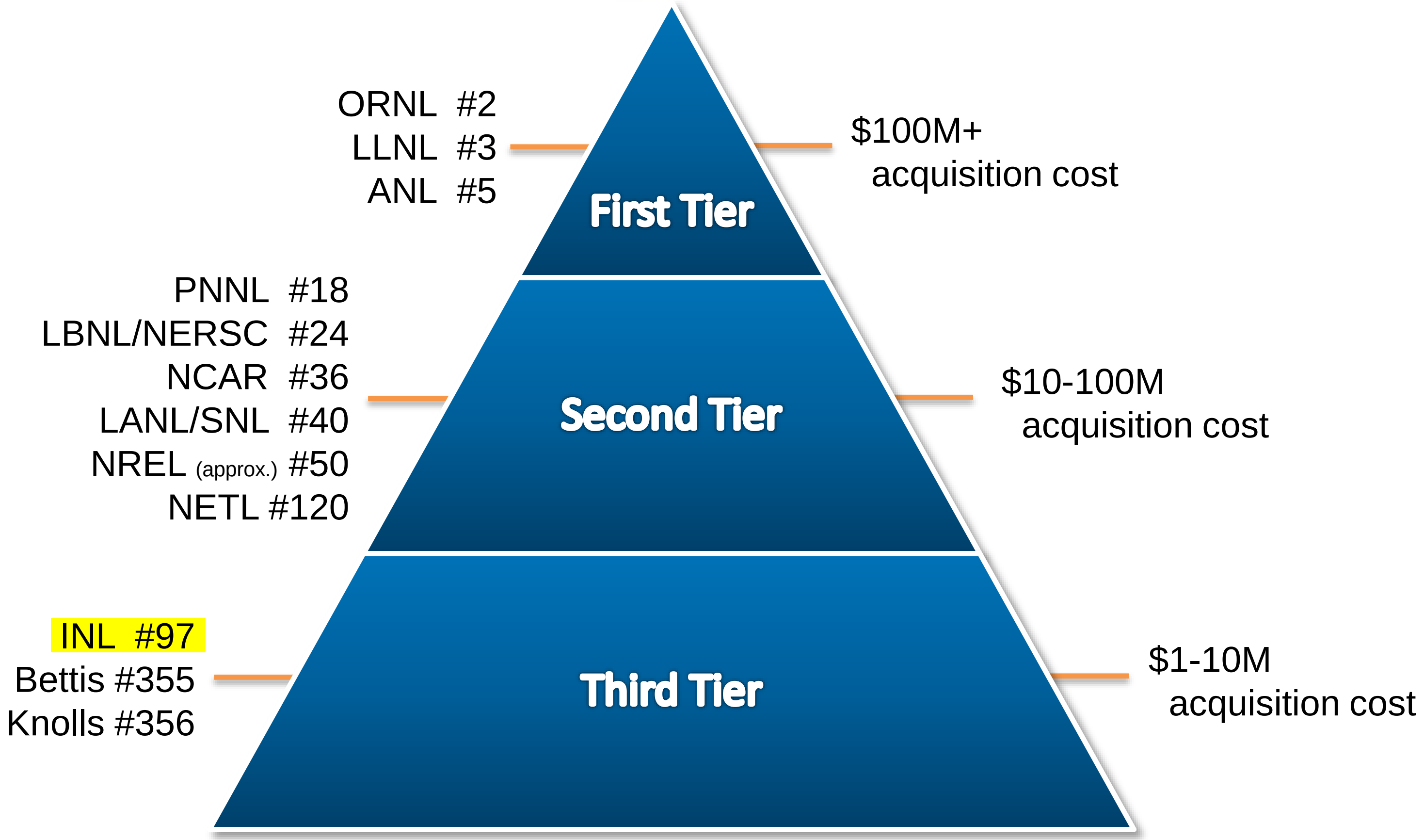


What does HPC hardware look like?

500 Teraflops per second
(multiplication of 500,000,000,000,000 numbers every second)

16,416 cores, 10 racks, 684 nodes
24 cores per node,128G RAM per node, Dual Xeon 2.5Ghz Intel Haswell
100 network switches, no hard disks, no connected graphics terminals, no keyboards

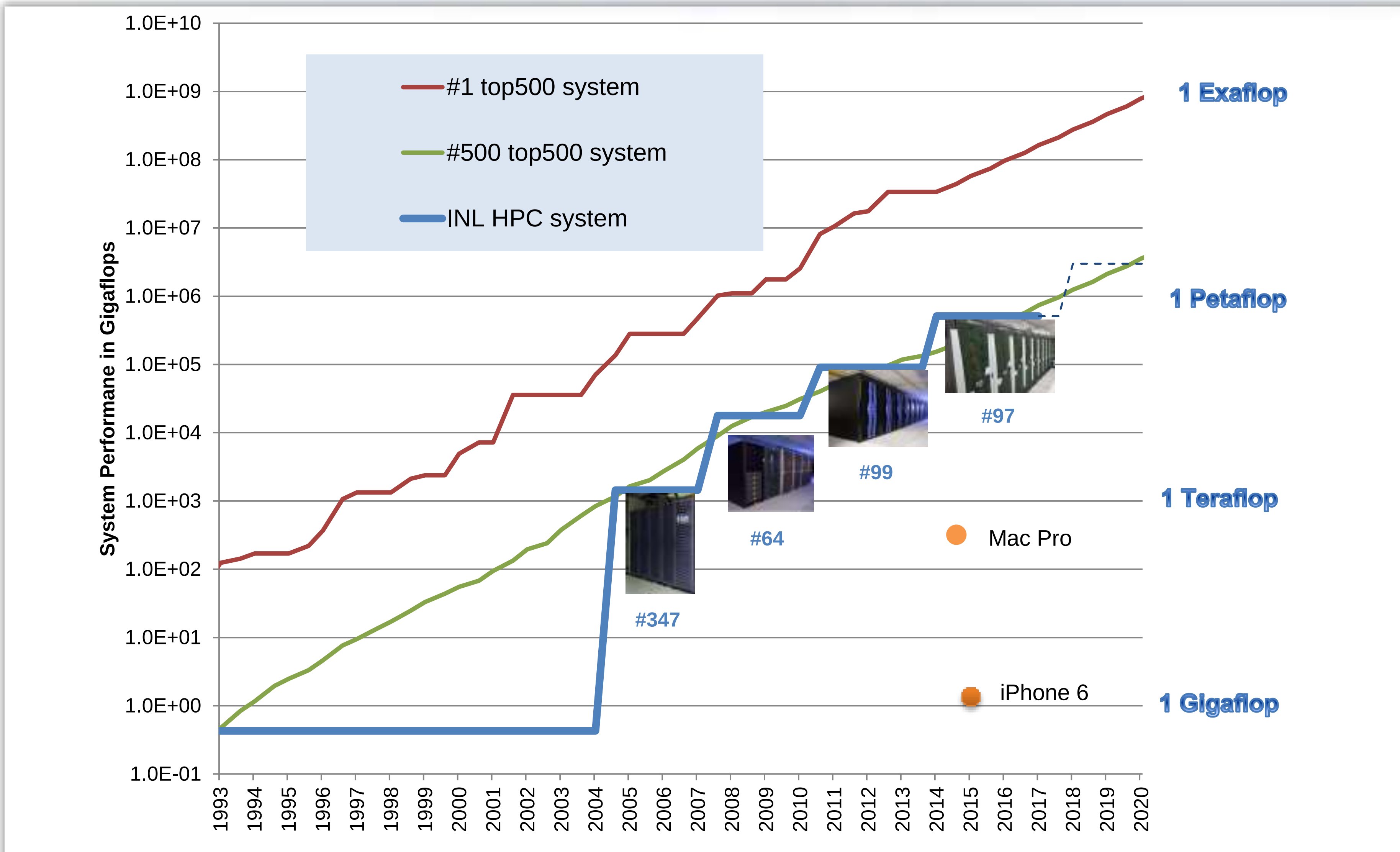
DOE Ecosystem – HPC Computing Systems



November 2014 Top500 Rankings

Approximately five systems in the first tier

HPC Trends – Top500 list

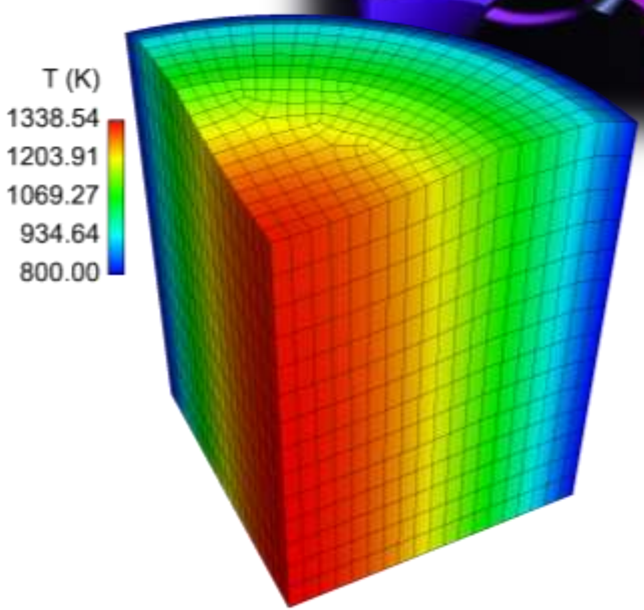


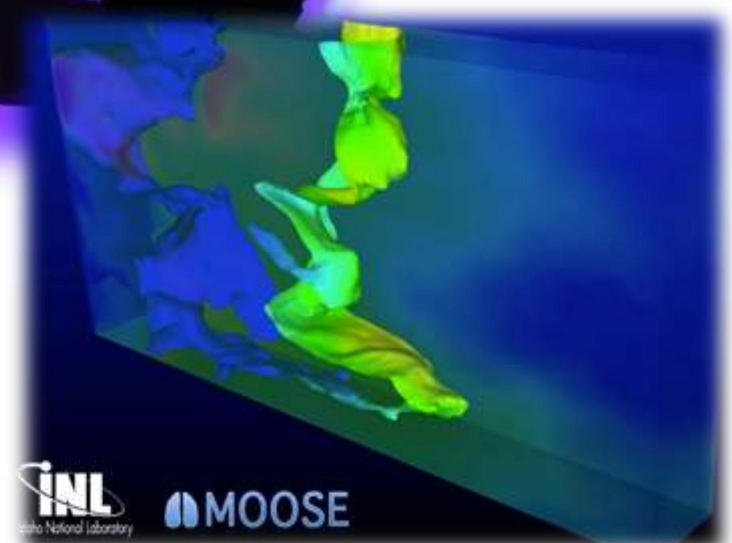
HPC Resources

HPC Systems	Architecture	Configuration
SGI Falcon 16,416 cores 87 TBytes memory	FDR Infiniband E5-2680v3 12 core 2.5GHz Haswell	684 nodes 24 cores/node 5.33 GB/core
Appro/Cray Fission 12,512 cores 25 TBytes memory	QDR Infiniband AMD 6136 8 core 2.4 GHz CPU	391 nodes 32 cores/node 2 GB/core

Storage Systems	Architecture	Configuration	Notes
EMC/Isilon	6 X400 primary NL400 Near store	1,210 Tbytes 12x10 Gbit/s	Home
Panasas	High speed parallel file system	240 TBytes 6x10Gbit/s	Scratch space

What does HPC software look like?





Terminology: models, numerical methods, simulation, verification and validation

- *Models* are mathematical expressions to approximate physics

$$\rho C p \frac{\partial T}{\partial t} - \nabla \cdot k(T, B) \nabla T = f$$

- *Numerical methods* approximately solve the models in space and time, typically with discretization procedures.
- *Simulation* employs software to apply the numerical methods over a given geometry (domain) for a chosen set of models.
- *Verification* is a mathematical/numerical process combined with “best software” practices (SQA) to provide confidence that the chosen models are being solved in a “mathematically correct” fashion (error control).
- *Validation* employs experiment to answer the question of whether the chosen models and numerical approach adequately represent the physics.

Importance of Integrating M&S with Experiment: It's a two-way street

How does experimental efforts benefit M&S?

- Verification and validation (V&V) of the software applications is necessary to provide for a simulation-based confidence.
- Without experiment, simulation of multiphysics phenomena becomes a useless exercise in mathematics and computer science.
- Typically, validation is an ongoing iterative process between M&S and experiment as the physical models are tuned and optimized to better replicate the phenomena being observed.
- In some instances, conducting experiments will result in discovering unknown phenomena for which mathematical models must be developed and then incorporated into software applications to increase predictive capability.

Computer Science & Mathematics + HPC Computational Framework

"The cornerstone of any HPC M&S effort"

- ***MOOSE:*** (Multi-physics Object-Oriented Simulation Environment), Derek Gaston
  - MOOSE makes INL's synergistic approach to multi-scale, multi-physics modeling & simulation possible.
  - INL's HPC development & runtime framework.
  - 1D, 2D or 3D FEM (CG, DG and XFEM) with both mesh and time step adaptivity.
  - Massively parallel, from 1 to 100,000's of processors.
  - Subjected to multiple peer-reviews and found to meet NQA-1 requirements.
  - Funding Source: LDRD (advanced development), NEAMS, CASL, and LWRS (program specific development).
  - Collaborators:

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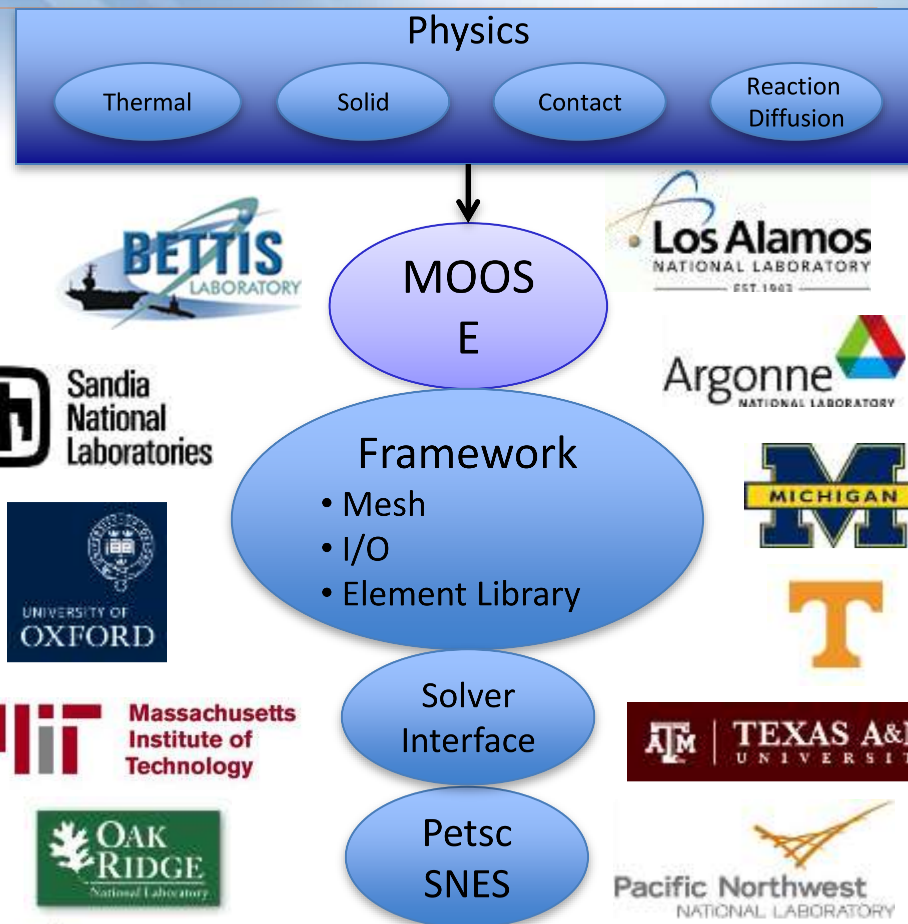
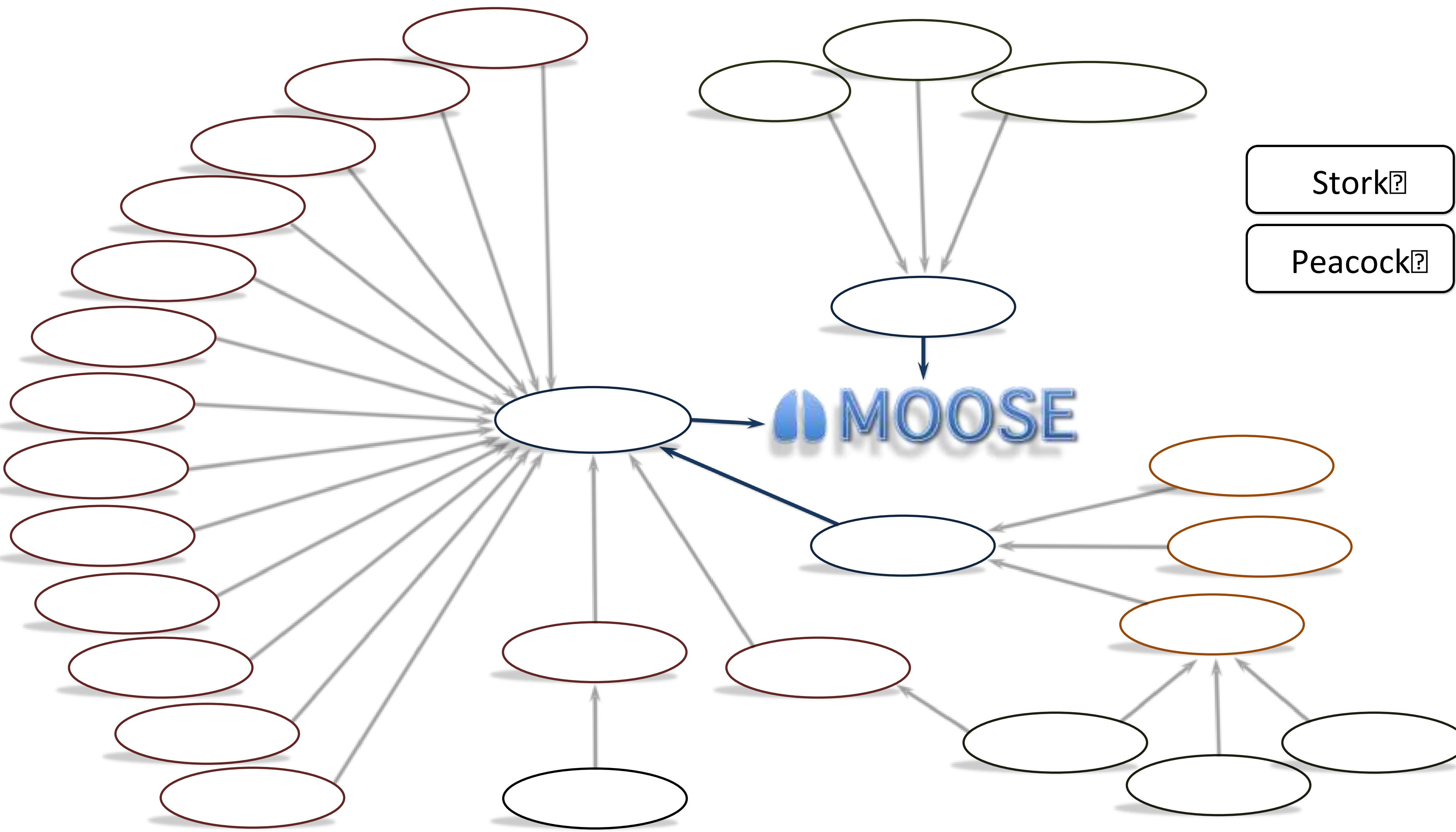
MOOSE Project

- MOOSE is an C++ object-oriented software framework allowing rapid development of new simulation tools.
- Leverages multiple DOE and university developed scientific computational tools.
- Derek Gaston received PECASE award for work on MOOSE (July of 2012).
- Obtained Free Software Foundation, Inc.'s Lesser General Public License Version 2.1on February 12, 2014.
- 2014 R&D 100 Award.
- Ecosystem of 30 known applications



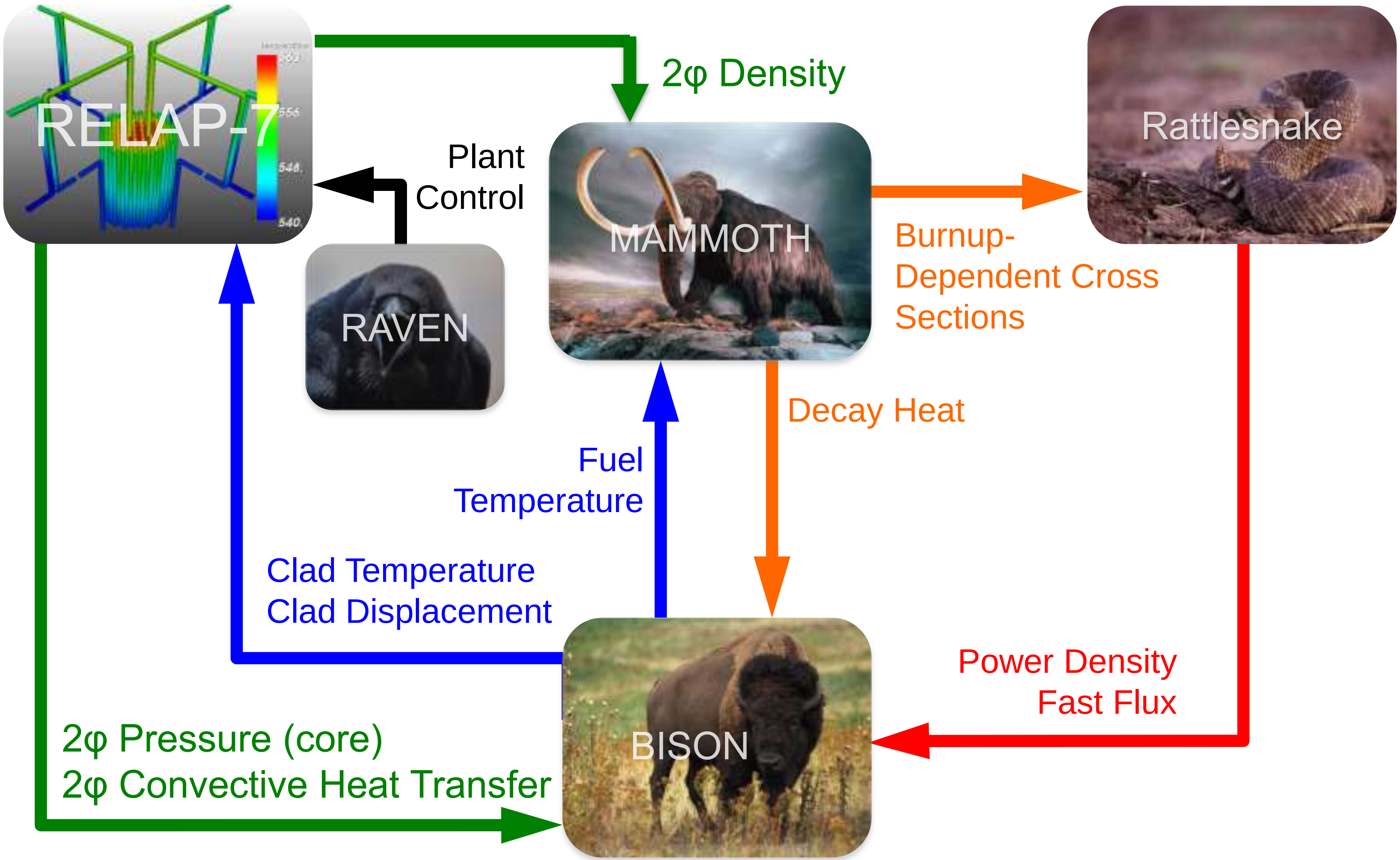
MOOSE Ecosystem



Stork

Peacock

This is what multi-physics fuels performance looks like



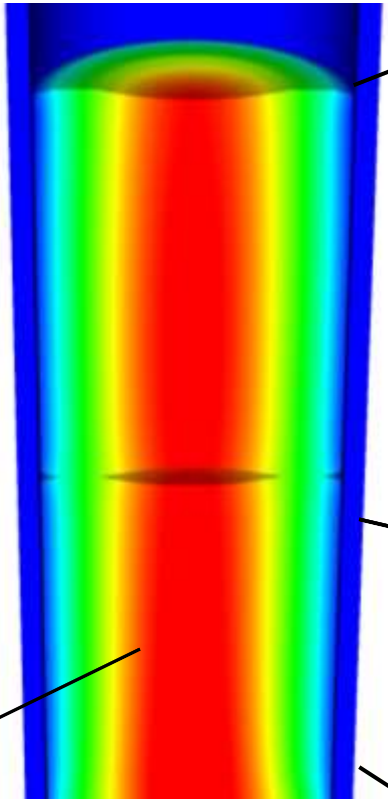
BISON Capabilities

General Capabilities

- Finite element based 1D spherical, 2D axisymmetric and 3D fully-coupled thermo-mechanics with species diffusion
- Linear or quadratic elements with large deformation mechanics
- Steady and transient operation
- Massively parallel computation
- Meso-scale informed material models

Oxide Fuel Behavior

- Temperature/burnup/porosity dependent conductivity
- Heat generation with radial and axial profiles
- Thermal expansion
- Solid and gaseous fission product swelling
- Densification
- Thermal and irradiation creep
- Fracture via relocation or smeared cracking
- Fission gas release (two stage physics)
  - transient (ramp) release
  - grain growth and grain boundary sweeping



Temperature

Gap/Plenum Behavior

- Gap heat transfer with k_g= f (T, n)
- Mechanical contact (master/slave)
- Plenum pressure as a function of:
  - evolving gas volume (from mechanics)
  - gas mixture (from FGR model)
  - gas temperature approximation

Cladding Behavior

- Thermal expansion
- Thermal and irradiation creep
- Irradiation growth
- Oxide layer growth
- Gamma heating
- Combined creep and plasticity
- Hydride damage

Coolant Channel

- Closed channel thermal hydraulics with heat transfer coefficients

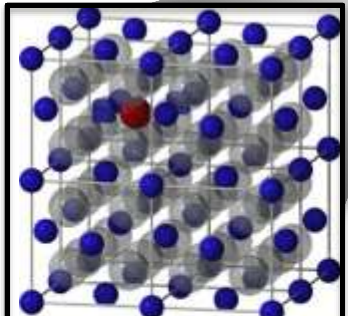
Solid Mechanics + Material Science

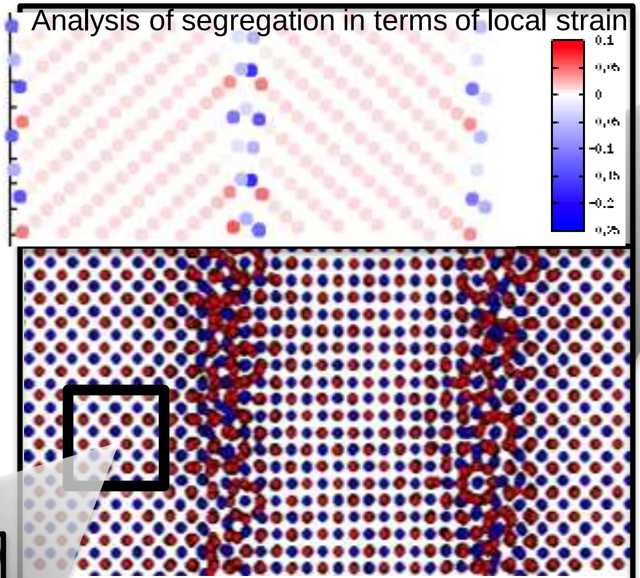
Multiscale Materials Modeling

- Develop advanced mechanistic materials models for reactor fuel, clad, CIs, and RPV using multi-scale modeling to enable predictive fuel performance simulations.

Atomic scale bulk DFT + MD

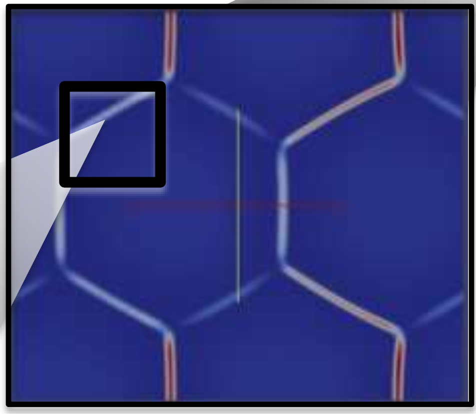
- Identify important bulk mechanisms
- Determine bulk material parameters





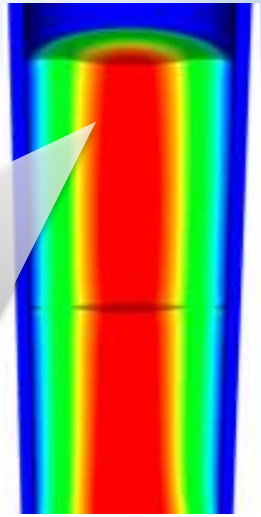
Atomic scale microstructure MD+DFT

- Investigate role of idealized interfaces
- Determine interfacial properties



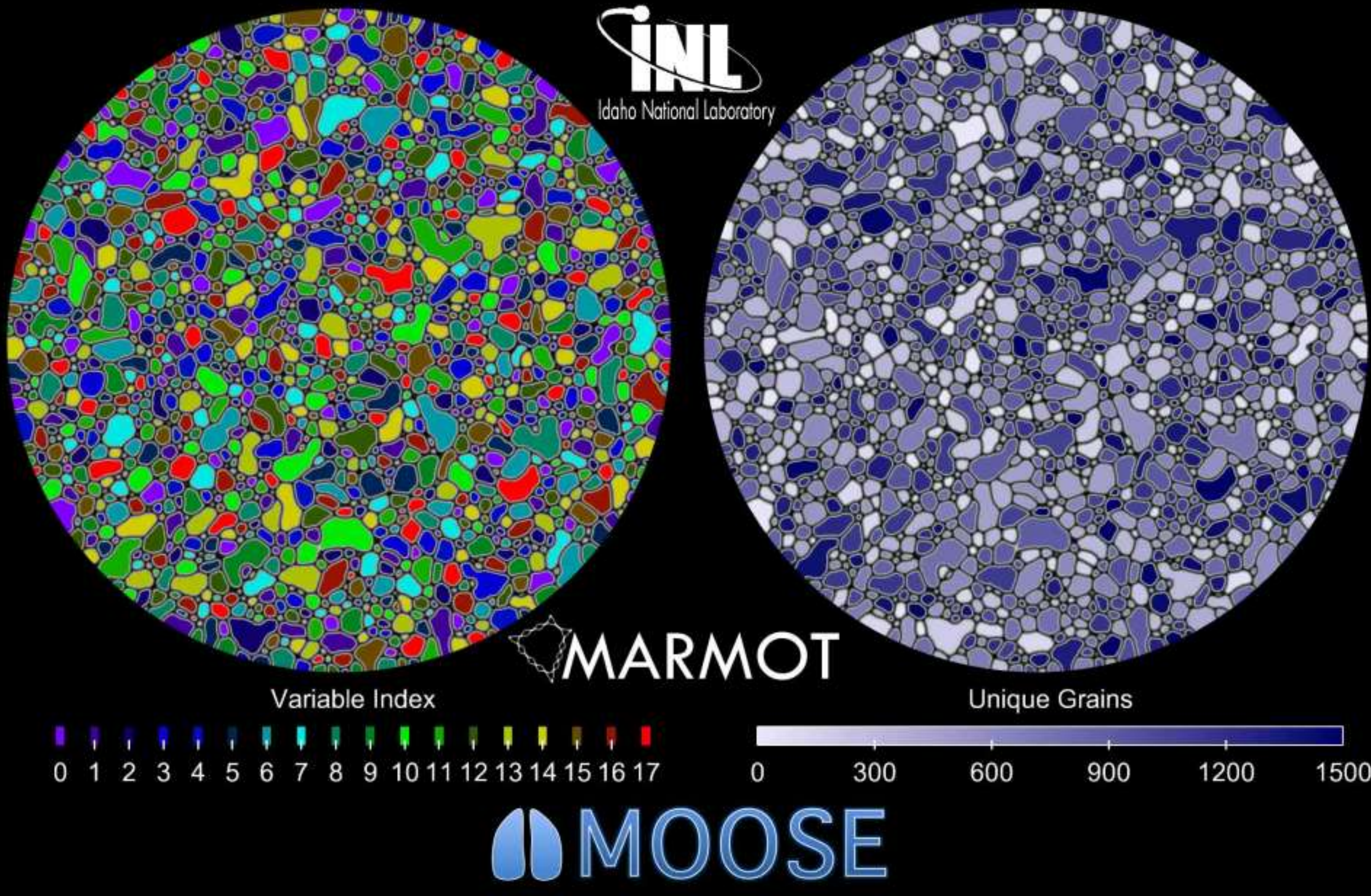
Mesoscale models (MARMOT)

- Predict and define microstructure state variable evolution
- Determine effect of evolution on material properties



Fuel performance models (BISON)

- Predict fuel performance during operation and accident conditions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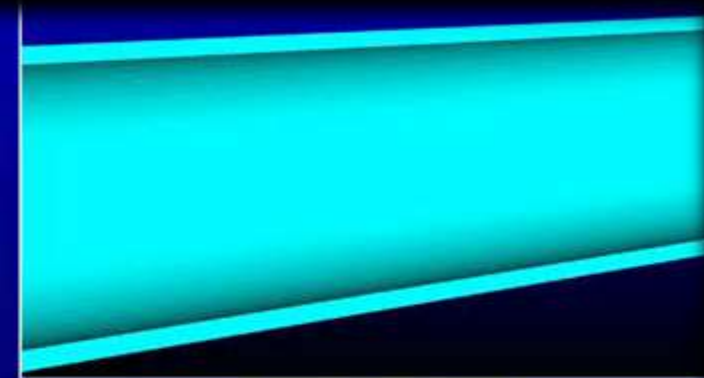
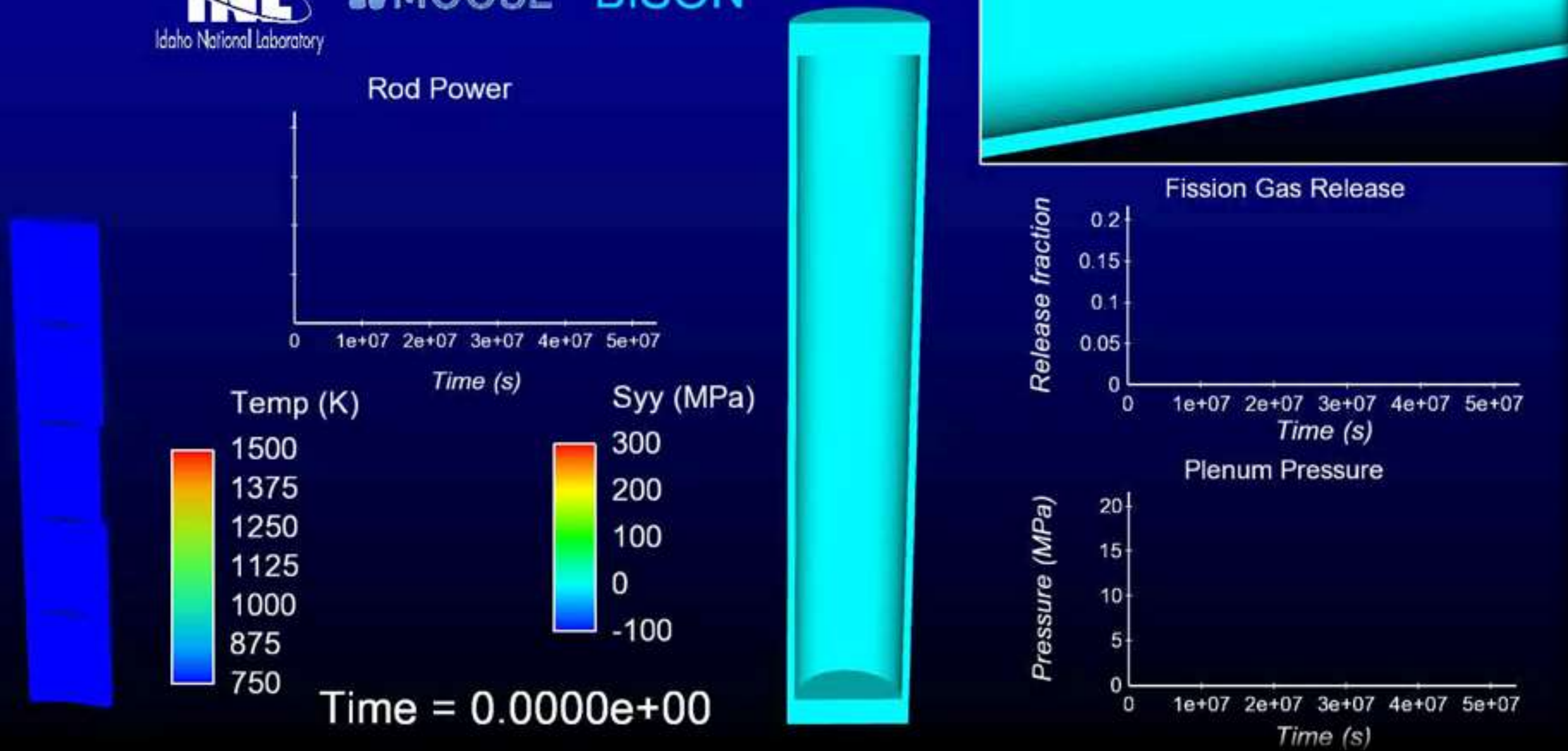
MARMOT
Variable Index
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
Unique Grains
0 300 600 900 1200 1500
MOOSE

Missing Pellet Surface

INL Idaho National Laboratory MOOSE BISON






MOOSE
RattleS$_N$ake RELAP-7 BISON
Time = 0.1 Days
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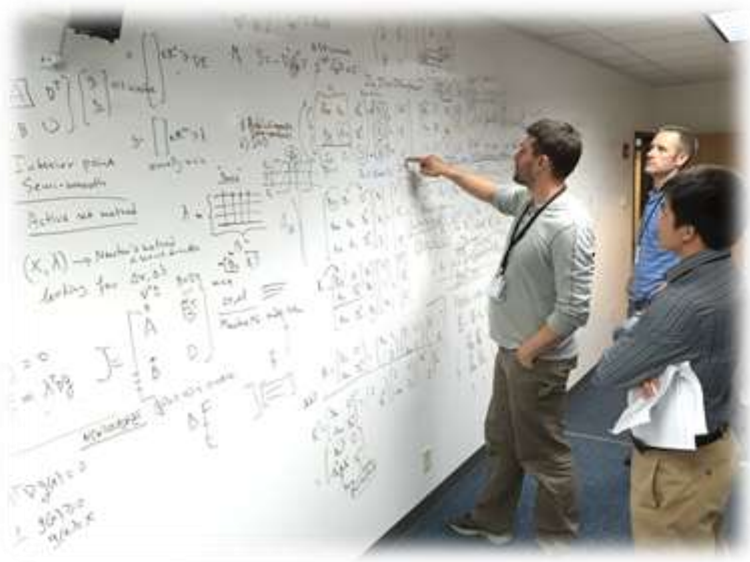
Temp.
1595
1332
1070
808
546

Collaborators Using HPC

Top 25 Collaborating Institutions
ORNL
University of Wisconsin
University of Michigan
University of Tennessee
University of Idaho
Westinghouse Electric Company
Boise State University
ANL
Core Physics Inc.
Ohio State University
USRA
Nuclear Regulatory Commission
Texas A&M University
Massachusetts Institute of Technology
Idaho State University
Oregon State University
LANL
BYU-Idaho
Universities Space Research Association
Universities Space Research Association
Washington State University
Pennsylvania State University
SNL
Seoul National University
University of South Carolina
North Carolina State University

	Projects in FY14
NEAMS	Nuclear Energy Advanced Modeling & Simulation
CASL	Center for Advanced Simulation of Light Water Reactors
IUC	Idaho University Consortium
NEUP	Nuclear Energy University Programs
CMSNF	Center for Material Science of Nuclear Fuels
ATR	Advanced Test Reactor
LWRS	Light Water Reactor Sustainability
EFRC	Energy Frontiers Research Center
PHISICS	Parallel and Highly Innovative Simulation for INL Code System
HFEF	INL's Hot Fuel Examination Facility Stack Analysis
GTRI	US High Power Research Reactor/Global Threat Reduction Initiative



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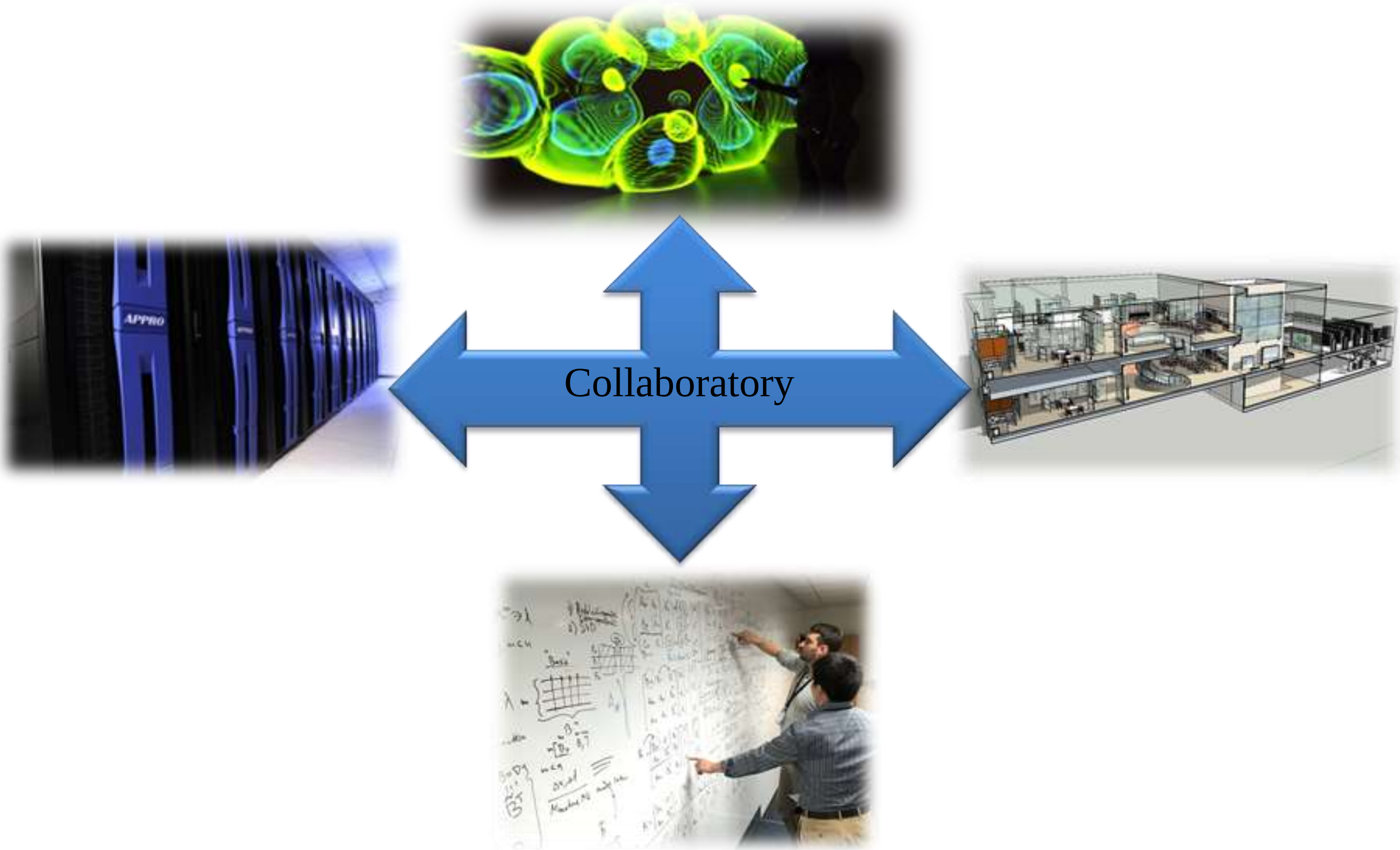


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